MULTIPLE ZETA VALUES AND ROTA–BAXTER ALGEBRAS

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Abstract. We study multiple zeta values and their generalizations from the point of view of Rota–Baxter algebras. We obtain a general framework for this purpose and derive relations on multiple zeta values from relations in Rota–Baxter algebras.

1. Introduction

The purpose of this paper is to establish the relationship between Rota–Baxter algebras and multiple zeta values, multiple polylogarithms and their q-analogs.

Multiple zeta values, henceforth abbreviated MZVs, are defined by

$$\zeta(s_1, \cdots, s_k) := \sum_{n_1 > n_2 > \cdots > n_k \geq 1} \frac{1}{n_1^{s_1} \cdots n_k^{s_k}} \tag{1}$$

where the s_i are positive integers with $s_1 > 1$.

The earliest algebraic relation among multiple zeta values traces back to Euler. Their systematic study started in early 1990s with the work of Hoffman [30] and Zagier [47]. Since then MZVs and their generalizations have been studied intensively by numerous authors with connections to arithmetic geometry, mathematical physics, quantum groups and knot theory. Surveys on the related work can be found in [7, 33, 10, 45, 46, 49]. Lately generalizations of MZVs, such as multiple polylogarithms (MPLs) have also been shown to be important, in both pure mathematics [47, 10] and theoretical physics [9, 35, 36]. Investigations of their possible q-analogs, especially with respect to algebraic aspects were started in [8, 43, 48, 49].

A Rota–Baxter operator of weight λ is a linear operator P on an algebra A such that

$$P(x)P(y) = P(xP(y)) + P(P(x)y) + \lambda P(xy),\ x, y \in A. \tag{2}$$

Here λ is a fixed constant in the base ring. Rota–Baxter algebra was first introduced by Baxter [5] in 1960 to study the theory of fluctuations in probability. It was further studied in the next two decades by a number of mathematicians, especially Rota who greatly contributed to the study of the Rota–Baxter algebra by his pioneering work in the late 1960s and early 1970s [38, 39, 40] and by his survey articles in late 1990s [41, 42].

In the last few years there have been further developments in Rota-Baxter algebras with applications to quantum field theory [12, 13, 21, 22, 23, 19, 15], dendriform algebras [1, 2, 3, 14, 17, 18], number theory [27], Hopf algebras [4, 16] and combinatorics [26]. Key to some of these developments in Rota–Baxter algebra is the realization of the free objects in which the product is defined by mixable shuffles [28, 29].

All known algebraic relations among MZVs are given by the combination of the shuffle product of the integral representation of MZVs and the stuffle (i.e., quasi-shuffle) product of the sum representation of the MZVs, and their degenerated forms. Conjecturally, all algebraic relations among MZVs can be obtained this way [34]. These products are also the shuffle product and mixable shuffle product in the free commutative Rota–Baxter algebras [28, 29, 16], as we will elaborate further below. It is therefore reasonable to expect that much of the recent work on algebraic relations for MZVs can be viewed and expanded in the framework of Rota–Baxter algebras. The current paper is a first step in this direction.

In order to make precise the connection between Rota–Baxter algebras and MZVs, and to set up a general framework to deal with the various generalizations of MZVs, we review the constructions of free commutative Rota–Baxter algebras in Section 2 and their relations with shuffle type products for MZVs. These include the relation between mixable shuffles in Rota–Baxter algebras and quasi-shuffles and generalized shuffles in MZVs, and the relation between the product of Cartier and stuffle product of MZVs. In Section 3, we use the language of free Rota–Baxter algebras to define the concept of MZV algebras which will include as special cases the MZVs, MPLs and q-MZVs. In Section 4, this setup is used to derive identities in MZVs from identities in Rota–Baxter algebras.

2. Free Rota-Baxter algebras and double shuffle

We start with reviewing the concept of free Rota–Baxter algebra because it most precisely and broadly relates Rota-Baxter algebras to MZVs. On one hand, the products in free Rota–Baxter algebras turn out to be the same as the products for MZVs. On the other hand, free Rota–Baxter algebras provide a general framework to define and study MZVs and their generalizations. Eventually, various classes of MZVs will be shown to be subquotients of free commutative Rota–Baxter algebras.

2.1. **Rota–Baxter algebras.** We first fix some notations. Throughout this paper, we will only consider commutative rings and algebras. For noncommutative Rota–Baxter algebras and applications to physics and operads, see [18, 19, 20, 23]. Let $\mathbf{k}$ be a unitary ring, that is, a ring with an identity which we denote by 1, and let $\lambda \in \mathbf{k}$ be fixed. A unitary (resp. nonunitary) Rota–Baxter $\mathbf{k}$-algebra (RBA) of weight λ is a pair (R, P) in which R is a unitary (resp. nonunitary) $\mathbf{k}$-algebra and $P : R \to R$ is a $\mathbf{k}$-linear map such that

$$P(x)P(y) = P(xP(y)) + P(P(x)y) + \lambda P(xy),\ \forall x,\ y \in R. \tag{3}$$

We will focus on two Rota-Baxter operators here. One is the integration operator

$$I(f)(x) = \int_0^x f(t)dt \tag{4}$$

defined on continuous functions $f(x)$ on $[0, \infty)$. Then the integration by parts formula reads

$$I(fI(g)) = I(f)I(g) - I(I(f)g)$$

showing that the integration operator is a Rota-Baxter operator of weight 0. The second operator is the sum operator that we will discuss at the beginning of the next section.

Let A be a unitary $\mathbf{k}$-algebra. A unitary Rota–Baxter algebra $(F(A), P_A)$ of weight λ is called a free unitary Rota–Baxter algebra over A if there is a unitary algebra homomorphism $j_A : A \to F(A)$ with the property that, for any unitary Rota–Baxter $\mathbf{k}$-algebra (R, P) of weight λ and unitary algebra homomorphism $f : A \to R$, there is a unitary Rota–Baxter

$\mathbf{k}$-algebra homomorphism $\bar{f} : (F(A), P_A) \to (R, P)$ such that $f = \bar{f} \circ j_A$, in other words, such that the diagram

$$\begin{tikzcd} A \arrow[r, "j_A"] \arrow[dr, "f"'] & F(A) \arrow[d, "\bar{f}"] \\ & R \end{tikzcd}$$

commutes. When all unitary is replaced by nonunitary in the above definition, we obtain the concept of the free nonunitary Rota-Baxter algebra over A.

2.2. **Free Rota-Baxter algebras and mixable shuffle product.** For a given unitary commutative algebra A, define $Ш^+(A) := \bigoplus_{n\geq 1} A^{\otimes n}$. We briefly recall the definition of **mixable shuffle product** $\diamond^+$ on $Ш^+(A)$. For details, see [16, 28, 29, 25].

Consider two pure tensors $a := a_1 \otimes \ldots \otimes a_m \in A^{\otimes m}$ and $b := b_1 \otimes \ldots \otimes b_n \in A^{\otimes n}$. As is well-known, a **shuffle** of a and b is a tensor permutation of a_i and b_j without changing the order of the a_is and b_js, and the shuffle product $aШb$ of a and b is the sum of shuffles of a and b. For example

$$a_1 Ш (b_1 \otimes b_2) = a_1 \otimes b_1 \otimes b_2 + b_1 \otimes a_1 \otimes b_2 + b_1 \otimes b_2 \otimes a_1.$$

More generally, a **mixable shuffle** is a shuffle in which some pairs $a_i \otimes b_j$ (but not $b_j \otimes a_i$) are merged into $\lambda a_i b_j$. The mixable shuffle product $a \diamond^+ b$ of a and b is the sum of mixable shuffles of a and b. For example,

$$a_1 \diamond^+ (b_1 \otimes b_2) = a_1 \otimes b_1 \otimes b_2 + b_1 \otimes a_1 \otimes b_2 + b_1 \otimes b_2 \otimes a_1 \quad \text{(shuffles)} \tag{5}$$
$$+\lambda a_1 b_1 \otimes b_2 + \lambda b_1 \otimes a_1 b_2 \quad \text{(merged shuffles)}. \tag{6}$$

So the mixable shuffle product is the shuffle product when $\lambda = 0$. With the product $\diamond^+$, $Ш^+(A)$ is a nonunitary commutative algebra. Let $\mathbf{k} \oplus Ш^+(A)$ be the unitary algebra after unitarization and let

$$Ш(A) := A \otimes (\mathbf{k} \oplus Ш^+(A))$$

be the tensor product algebra with its product denoted by $\diamond$. So for $a \otimes (u + a')$ and $b \otimes (v + b')$ in $Ш(A)$ with $a, b \in A$, $u, v \in \mathbf{k}$ and $a', b' \in Ш^+(A)$, we have the product

$$(a \otimes a') \diamond (b \otimes b') = (ab) \otimes (uv + va' + ub' + a' \diamond^+ b'). \tag{7}$$

We have the natural unitary algebra homomorphism $j_A : A \to Ш(A)$ sending $a \in A$ to $a \otimes 1 \in Ш(A)$. The following theorem is proved in [28, 29].

Theorem 2.1. *The algebra $Ш(A)$ with the shift operator $P_A : Ш(A) \to Ш(A), P_A(a) := 1 \otimes a$ is the free commutative unitary Rota–Baxter algebra over A. When $A = \mathbf{k}[X]$, it is the free commutative unitary Rota-Baxter algebra over X.*

If A is a nonunitary algebra, then the free commutative nonunitary algebra over A can be constructed as a subalgebra of $Ш(\tilde{A})$ [29]. Here $\tilde{A} = \mathbf{k} \oplus A$ is the unitarization of A.

2.3. **Connection with quasi-shuffle.** It is shown in [16] that the mixable shuffle product can be recursively defined as follows. For any $m, n \geq 1$ and $a = a_1 \otimes \cdots \otimes a_m \in A^{\otimes m}$, $b = b_1 \otimes \cdots \otimes b_n \in A^{\otimes n}$, then

$$a \diamond^+ b = \begin{cases} a_1 \otimes b_1 + b_1 \otimes a_1 + \lambda a_1 b_1, & m = n = 1, \\ a_1 \otimes b_1 \otimes \cdots \otimes b_n + b_1 \otimes \big(a_1 \diamond^+ (b_2 \otimes \cdots \otimes b_n)\big) \\ \qquad\qquad + \lambda (a_1 b_1) \otimes b_2 \otimes \cdots \otimes b_n, & m = 1, n \geq 2, \\ a_1 \otimes \big((a_2 \otimes \cdots \otimes a_m) \diamond^+ b_1\big) + b_1 \otimes a_1 \otimes \cdots \otimes a_m \\ \qquad\qquad + \lambda (a_1 b_1) \otimes a_2 \otimes \cdots \otimes a_m, & m \geq 2, n = 1, \\ a_1 \otimes \big((a_2 \otimes \cdots \otimes a_m) \diamond^+ (b_1 \otimes \cdots \otimes b_n)\big) \\ \qquad + b_1 \otimes \big((a_1 \otimes \cdots \otimes a_m) \diamond^+ (b_2 \otimes \cdots \otimes b_n)\big) \\ \qquad\qquad + \lambda (a_1 b_1) \otimes \big((a_2 \otimes \cdots \otimes a_m) \diamond^+ (b_2 \otimes \cdots \otimes b_n)\big), & m, n \geq 2. \end{cases} \tag{8}$$

This is a mild generalization of the quasi-shuffle product introduced by Hoffman [32] at about the same time as the mixable shuffle product to study MZVs. We briefly recall his construction. Let X be a set with a grading given by finite subsets $X_n, n \geq 1$, (locally finite set) and with either a graded associative commutative product $[\cdot, \cdot] : X \times X \to X$ or the zero product $[\cdots, \cdots] : X \times X \to \{0\}$. Let $\mathfrak{A}$ be the noncommutative free algebra on X with identity 1. Elements in X are called letters and monomials in $\mathfrak{A}$ are called words. Hoffman's **quasi-shuffle product** is the product $*$ on $\mathfrak{A}$ recursively defined by

(1) $1 * w = w * 1 = w$ for any word w;
(2) $(aw_1) * (bw_2) = a(w_1 * (bw_2)) + b((aw_1) * w_2) + [a, b](w_1 * w_2)$, for any words w_1, w_2 and letters a, b.

Then $(\mathfrak{A}, *)$ is a commutative algebra. We thus have [16]

Theorem 2.2. *The products $*$ coincides with $\diamond^+$ on $Ш^+(A)$ in the special case when $\lambda = 1$ and when A is the algebra $\mathbf{k} \oplus (\oplus_{x \in X} \mathbf{k}x)$ with product given by $[\cdot, \cdot]$.*

The mixable shuffle product was also found by Goncharov [24] in the context of motivic shuffle relations.

As another interesting link between Rota–Baxter algebras and MZVs, we note that a construction of free Rota–Baxter algebras over a set was obtained over 30 years ago by Cartier [11] where the product is defined in terms of ordered subsets. Recently [8] the stuffle product for MZVs was described in a similar way using order preserving injections instead of ordered subsets.

3. Rota–Baxter algebra setup of MZVs and their generalizations

The above section gives strong evidence on the intrinsic connection between Rota–Baxter algebra and MZVs. In order to effectively apply results of Rota–Baxter algebras to MZVs, it is desirable to give a Rota–Baxter algebra structure on the set of MZVs. As we see in Eq (1), the MZVs are defined by iterated sums, given by iterations of the sum operator

$$P(f)(x) := \sum_{n \geq 1} f(x + n).$$

Under certain convergency conditions, such as $f(x) = O(x^{-2})$ and $g(x) = O(x^{-2})$, $P(f)(x)$ and $P(g)(x)$ are defined by absolutely convergent series and we have

$$\begin{aligned} P(f)(x)P(g)(x) &= \sum_{m\geq 1} f(x+m) \sum_{n\geq 1} g(x+n) \\ &= \sum_{n>m\geq 1} f(x+m)g(x+n) + \sum_{m>n\geq 1} f(x+m)g(x+n) + \sum_{m\geq 1} f(x+m)g(x+m) \\ &= P(fP(g))(x) + P(gP(f))(x) + P(fg)(x) \end{aligned} \tag{9}$$

since

$$\begin{aligned} P(fP(g))(x) &= \sum_{m=1}^{\infty} f(x+m)P(g)(x+m) \\ &= \sum_{m=1}^{\infty} f(x+m)\big(\sum_{k=1}^{\infty} g(x+m+k)\big) \\ &= \sum_{n>m\geq 1} f(x+m)g(x+n). \end{aligned}$$

This shows that the operator P is a Rota-Baxter operator of weight 1 on certain functions. However, the sum operator and its iteration are not defined on some other functions. So we can only expect that subsets of a Rota–Baxter algebra can be applied to the MZV study. This motivates the following construction.

3.1. MZV algebras.

Let R be a $\mathbf{k}$-algebra. Let P be a partially defined map from R to R. We call P a partially defined Rota–Baxter operator if

$$P(f)P(g) = P(fP(g)) + P(P(f)g) + \lambda P(fg) \tag{10}$$

if all terms are defined.

For $\mathbf{f} := (f_1, \cdots, f_n) \in R^n$, formally define

$$P_{\mathbf{f}} := P(f_1 P(f_2 \cdots P(f_n) \cdots)).$$

We define a **filtered k-algebra** to be a nonunitary $\mathbf{k}$-algebra A with a decreasing sequence $A_n, n \geq 0$, of ideals such that $A_m A_n \subseteq A_{m+n}$.

Definition 3.1. *Let R be a $\mathbf{k}$-algebra with a partially defined Rota–Baxter operator P. A filtered subalgebra A of R is called* **iteratedly summable** *(of level k) if the formal symbols $P_{\mathbf{f}}$ are well-defined for all $\mathbf{f} \in A^n$, $n \geq 1$, with $f_n \in A_k$. For an iteratedly summable subalgebra A (of level k), we call the set*

$$\mathfrak{A}_k := \{P_{(f_1,\cdots,f_n)} \big| f_i \in A, 1 \leq i \leq n, f_n \in A_k\}$$

the **MZV algebra** *generated by A.*

We will show below (Theorem 3.2) that $\mathfrak{A}_k$ is indeed an algebra.

3.2. **The abstract MZV algebra.** Let A be a filtered $\mathbf{k}$-algebra. We can construct a MZV-algebra generated by A as follows.

Let $\tilde{A}$ be the unitarization of A. So $\tilde{A} = \mathbf{k} \oplus A$ with componentwise addition and with product defined by $(m,a)(n,b) = (mn, mb+na+ab)$. In the free Rota–Baxter algebra $Ш(\tilde{A})$ with Rota-Baxter operator P_A, we have $P_A(f) = 1 \otimes f$. So $P_{A,(f_1,\cdots,f_n)} = 1 \otimes f_1 \otimes \cdots f_n$. Therefore, for $k \geq 1$, the MZV algebra generated by A in $Ш(\tilde{A})$ is the subspace $\mathfrak{M}(A)_k$ of $Ш(\tilde{A})$ generated by pure tensors of the form $1 \otimes a_1 \otimes \cdots \otimes a_n \in 1 \otimes A^{\otimes n}$ with $a_n \in A_k$.

Theorem 3.2. *Let A be an iteratedly summable subalgebra of R of level k.*

1. $\mathfrak{A}_k$ *is a subalgebra of R.*
2. $\mathfrak{M}(A)_k$ *is a subalgebra of* $Ш(\tilde{A})$.
3. *There is an algebra surjection*
$$\mathfrak{P}_k : \mathfrak{M}(A)_k \to \mathfrak{A}_k$$
sending $1 \otimes f_1 \otimes \cdots \otimes f_n$ *to* $P_{(f_1,\cdots,f_n)}$.
4. *Given an evaluation, that is, an algebra homomorphism $\nu : A \to \mathbf{k}$, we obtain an algebra homomorphism $\nu \circ \mathfrak{P}_k : \mathfrak{M}(A)_k \to \mathbf{k}$.*

Proof. (1) We only need to prove that $\mathfrak{A}$ is closed under multiplication. For this we just need to prove that for any $(f_1,\cdots,f_m) \in A^m$, $(g_1,\cdots,g_n) \in A^n$ with $f_i, g_j \in A$ and $f_m, g_n \in A_k$, the product $P_{(f_1,\cdots,f_m)}P_{(g_1,\cdots,g_n)}$ are still of this form. We prove this by induction on $m+n$. When $m = n = 1$, we have $f_1, g_1 \in A_k$. Then

$$\begin{aligned} P_{f_1}P_{g_1} &= P(f_1)P(g_1) \\ &= P(f_1P(g_1)) + P(g_1P(f_1)) + \lambda P(f_1g_1). \end{aligned}$$

So we are done. Assuming the claim is true for $m+n \leq k$ and consider the case of $m+n = k+1$. Then the Rota-Baxter relation (10)

$$\begin{aligned} P_{(f_1,\cdots,f_m)}P_{(g_1,\cdots,g_n)} &= P(f_1P_{(f_2,\cdots,f_m)})P(g_1P_{(g_2,\cdots,g_n)}) \\ &= P(f_1P_{(f_2,\cdots,f_m)}P(g_1P_{(g_2,\cdots,g_n)})) + P(P(f_1P_{(f_2,\cdots,f_m)})g_1P_{(g_2,\cdots,g_n)}) \\ &\quad +\lambda P(f_1P_{(f_2,\cdots,f_m)}g_1P_{(g_2,\cdots,g_n)}). \end{aligned}$$

By the induction hypothesis, $P_{(f_2,\cdots,f_m)}P(g_1P_{(g_2,\cdots,g_n)}) = P_{(f_2,\cdots,f_m)}P_{(g_1,\cdots,g_n)}$ is a sum of terms of the form $P_{(h_1,\cdots,h_\ell)}$ with $h_i \in A$ and $h_\ell \in A_k$. So $P(f_1P_{(f_2,\cdots,f_m)}P(g_1P_{(g_2,\cdots,g_n)}))$ is also a sum of the form $P_{(f_1,h_1,\cdots,h_\ell)}$, so are still in $\mathfrak{A}_k$. The same argument applies to the other two terms. This completes the induction.

(2) By construction, $\mathfrak{M}(A)$ is a special case of $\mathfrak{A}_k$.

(3) The assigned map is clearly well-defined and surjective. It is an algebra homomorphism because the products in $\mathfrak{M}(A)$ and $\mathfrak{A}_k$ are both defined by the Rota-Baxter relation (10). Alternatively, it can be proved by induction, as in item (1).

(4) follows from item (3) since a composition of algebra homomorphisms is still an algebra homomorphism. □

Corollary 3.3. *If F is an algebraic relation among elements $f_i, 1 \leq i \leq n$ in $\mathfrak{M}(A)_k$ for a given k, then $\mathfrak{P}_k(F)$ gives the same algebraic relation among the elements $\mathfrak{P}_k(f_i), 1 \leq i \leq n$ in the MZV algebra $\mathfrak{A}_k$ and the same algebraic relation among elements $(\nu \circ \mathfrak{P}_k)(f_i), 1 \leq i \leq n$ of $\mathbf{k}$.*

3.3. **Examples of MZV algebras.** As we have seen at the beginning of this section, for the sum operator $P(f)(x) = \sum_{n=1}^{\infty} f(x+n)$, we have

$$P_{(f_1,\cdots,f_k)}(x) = \sum_{n_1>n_2>\cdots>n_k\geq 1} f_1(x+n_1)f_2(x+n_2)\cdots f_k(x+n_k) \tag{11}$$

under suitable convergence condition.

3.3.1. *Multiple Hurwitz zeta functions and MZVs.* We let

$$A_H := \{f_s(x) := 1/x^s \big| s \in \mathbb{N}\}$$

with filtration given by s. Then A_H is a filtered subalgebra and generates a MZV algebra. More precisely, we have

$$P(f_s)(x) = \sum_{n=1}^{\infty} \frac{1}{(x+n)^s} = \zeta(s; x+1)$$

where $\zeta(s;x)$ is the Hurwitz zeta function [10]. Evaluated at $x=0$, we obtain the Riemann zeta function $\zeta(k)$.

We define a **multiple Hurwitz zeta function** to be an iteration

$$\zeta(s_1,\cdots,s_k; x+1) := P_{(f_{s_k},\cdots,f_{s_1})}(x) = \sum_{n_1>n_2>\cdots>n_k\geq 1} \frac{1}{(x+n_1)^{s_1}\cdots(x+n_k)^{s_k}}$$

with $s_1 > 1$. So the MZV algebra $\mathfrak{A}_H$ of level 2 generated by A_H is the algebra of multiple Hurwitz zeta functions.

Taking the evaluation map $\nu(f(x)) = f(0)$, we obtain the algebra of multiple zeta values

$$\zeta(s_1,\cdots,s_k) := \sum_{n_1>n_2>\cdots>n_k\geq 1} \frac{1}{n_1^{s_1}\cdots n_k^{s_k}}.$$

For example, for $P(f_2)(x) = \sum_{n=1}^{\infty} \frac{1}{(x+n)^2} = \zeta(2;x+1)$, by the Rota-Baxter relation (9), we have $P(f_2)P(f_2) = P(f_2P(f_2)) + P(P(f_2)f_2) + P(f_2f_2)$. Since $f_2f_2 = f_4$, we obtain

$$\zeta(2;x+1)\zeta(2;x+1) = 2\zeta(2,2;x+1) + \zeta(4;x+1).$$

Evaluating at $x=0$, we obtain

$$\zeta(2)\zeta(2) = 2\zeta(2,2) + \zeta(4). \tag{12}$$

Further applications of Rota-Baxter algebras to MZVs will be given in the next section.

3.3.2. *Multiple Lerch functions and MPLs.* Now let $s \in \mathbb{N}$ and z be a (complex) parameter with $|z| < 1$. Let

$$A_L := \{f_{s,z}(x,y) := z^y/x^s \big| s \in \mathbb{N}, |z| < 1\}.$$

Then A_L is a filtered algebra from the grading by s. We have

$$P(f_{s,z})(x,y) := \sum_{n=1}^{\infty} \frac{z^{y+n}}{(x+n)^s}$$

and $P(f_{s,z})(x,0) = \Phi(z,s,x+1)$ where $\Phi(z,s,x)$ is the Lerch function [10]. Evaluated at $x=0$, we obtain the polylogarithm function

$$Li_s(z) := \sum_{n\geq 1} \frac{z^n}{n^s}.$$

Further $Li_s(1)$ is the Riemann zeta function.

We define a **multiple Lerch function** to be an iteration

$$\zeta(s_1, \cdots, s_k; x+1) := P_{(f_{s_1,z_1}, \cdots, f_{s_k,z_k})}(x,y) = \sum_{n_1>n_2>\cdots>n_k\geq 1} \frac{z_1^{y+n_1}\cdots z_k^{y+n_k}}{(x+n_1)^{s_1}\cdots(x+n_k)^{s_k}}.$$

So the MZV algebra $\mathfrak{A}_L$ generated by A_L is the algebra of multiple Lerch functions.

When $y = x = 0$, we obtain the multiple polylogarithms

$$Li_{s_1,\cdots,s_k}(z_1, \cdots, z_k) := \sum_{n_1>n_2>\cdots>n_k\geq 1} \frac{z_1^{n_1}\cdots z_k^{n_k}}{n_1^{s_1}\cdots n_k^{s_k}}.$$

3.3.3. *Variations of q-MZVs.* There are several versions of q-MZVs and q-MPLs. See [48, 8] for q-multiple zeta values and polylogarithms. See also [49] for another definition of q-MZVs. They can all be defined as iterations of summation operators on certain functions.

Fix $0 < q < 1$ Let A_q be the subspace with basis

$$\left\{ \mathfrak{q}_s(k) := \frac{q^{k(s-1)}}{[k]_q^s} \;\middle|\; s \in \mathbb{C} \right\}.$$

Here $[k]_q = \frac{1-q^k}{1-q}$. Then A_q is a filtered subalgebra since

$$\mathfrak{q}_s(k)\mathfrak{q}_t(k) = \mathfrak{q}_{s+t}(k) + (1-q)\mathfrak{q}_{s+t-1}(k).$$

The MZV algebra $\mathfrak{A}_{q,2}$ of level 2 generated by A_q, after the evaluation map, is the algebra of q-MZVs studied by Zhao, Bradley, Kaneko, et. al. [48, 8, 37] consisting elements of the form

$$\zeta_q(s_1, \cdots, s_d) := \sum_{k_1>\cdots>k_d>0} \frac{q^{k_1(s_1-1)+\cdots+k_d(s_d-1)}}{[k_1]^{s_1}\cdots[k_d]^{s_d}} \tag{13}$$

where $s_1 > 1$.

3.4. **Rota–Baxter algebras and nested sums.** There is another angle to the Rota–Baxter algebra point of view for MZVs. Let A be a unitary ring and let $\mathbb{N}$ be the set of positive integers. Define $\mathcal{A} := \mathrm{Map}(\mathbb{N}, A) = A^{\mathbb{N}}$ to be the algebra of maps $f : \mathbb{N} \to A$ with point-wise operations. Define a linear operator

$$Z := Z_{\mathcal{A}} : \mathcal{A} \to \mathcal{A}, \quad Z[f](k) := \begin{cases} \sum_{i=1}^{k-1} f(i), & k > 1, \\ 0, & k = 1. \end{cases} \tag{14}$$

Lemma 3.4. *Z is a Rota–Baxter operator on $\mathcal{A}$ of weight 1.*

Further we have, for $f_1, \cdots, f_n \in \mathcal{A}$,

$$Z[f_1 Z[f_2 \cdots Z[f_n] \cdots]](k+1) = \sum_{k\geq i_1>\cdots>i_n>0} f_1(i_1)\cdots f_n(i_n) \tag{15}$$

and thus

$$\lim_{k\to\infty} Z[f_1 Z[f_2 \cdots Z[f_n] \cdots]](k) = \sum_{i_1>\cdots>i_n>0} f_1(i_1)\cdots f_n(i_n) \tag{16}$$

if the nested infinite sum on the right exists.

For example, the multiple zeta values are obtained as

$$\zeta(s_1,\cdots,s_n)=\sum_{i_1>\cdots>i_n>0}\frac{1}{i_1^{s_1}\cdots i_n^{s_n}}=\lim_{k\to\infty}Z\Big[\frac{1}{x^{s_1}}Z\Big[\frac{1}{x^{s_2}}\cdots Z\Big[\frac{1}{x^{s_n}}\Big]\cdots\Big]\Big](k).$$

3.5. **Rota–Baxter algebras and iterated integrals.** We mentioned in the introduction the double-shuffle relations for MZVs, corresponding to the sum and integral representations of MZVs (see [34] for more details). We have just seen that the sum representation of MZVs is captured as a subquotient A_H of a free Rota-Baxter algebra of weight 1 (Theorem 3.2). Similarly, the integral representation of MZVs is captured by a Rota-Baxter algebra of weight zero, the integral operator considered in Eq (4). For example the integral representation

$$\zeta(2)=\int_0^1\frac{dx_1}{x_1}\int_0^{x_1}\frac{dx_2}{1-x_2}$$

is the evaluation at $x=1$ of

$$I_{(1/x_1,1/(1-x_2))}:=\int_0^x\frac{dx_1}{x_1}\int_0^{x_1}\frac{dx_2}{1-x_2}$$

for the integration operator I in Eq. (4) which is a Rota-Baxter operator of weight zero. Since the product in a free Rota-Baxter algebra of weight zero is given by the shuffle product, we have

$$\begin{aligned}I_{(1/x_1,1/(1-x_2))}I_{(1/y_1,1/(1-y_2))} &= I_{(1/x_1,1/y_1,1/(1-x_2),1/(1-y_2))}+I_{(1/x_1,1/y_1,1/(1-y_2),1/(1-x_2))}\\ &\quad +I_{(1/y_1,1/x_1,1/(1-x_2),1/(1-y_2))}+I_{(1/y_1,1/x_1,1/(1-y_2),1/(1-x_2))}\\ &\quad +I_{(1/x_1,1/(1-x_2),1/y_1,1/(1-y_2))}+I_{(1/y_1,1/(1-y_2),1/x_1,1/(1-x_2))}\\ &= 4I_{(1/z_1,1/z_2,1/(1-z_3),1/(1-z_4))}+2I_{(1/z_1,1/(1-z_2),1/z_3,1/(1-z_4))}.\end{aligned}$$

Evaluated at $x=1$, we have

$$\zeta(2)\zeta(2)=4\zeta(3,1)+2\zeta(2,2).$$

Combining with Eq (12) we have the famous relation

$$\zeta(3,1)=\frac{1}{4}\zeta(4).$$

In general, this double-shuffle structure is reflected in the context of Rota-Baxter algebras and needs to be further analyzed.

We will only briefly mention the integral representation of q-MZVs, as they appeared in [48, 8]. The q-analog of the Riemann integral, named Jackson integral after its inventor Reverend Jackson [42], on a well chosen function algebra is given by

$$J[f](x):=\int_0^x f(y)d_qy:=(1-q)\sum_{n\geq 0}f(xq^n)xq^n. \tag{17}$$

for $0<q<1$. A key ingredient in the Jackson integral is the operator

$$P_q[f](x):=\sum_{n>0}f(xq^n). \tag{18}$$

Proposition 3.5. [41] *The maps P_q and $\hat{P}_q:=id+P_q$ are Rota-Baxter operators of weight 1 and -1, respectively.*

It then follows that Jackson's integral satisfies the relation

$$J[f]\,J[g] + (1-q)J[f\,g\,\mathrm{id}] = J\Big[J[f]\,g + f\,J[g]\Big], \tag{19}$$

where id is the identity map.

The q-analogs of MZVs of [48, 8] have a Jackson-integral representation. Unfortunately, Theorem 3.2 does not apply to the integral representation of these q-MZVs due to the lack of a suitable MZV algebra structure here. We plan to elaborate on this in a future work.

4. Identities in Rota–Baxter algebras and MZVs

By Corollary 3.3, once we have an identity in free Rota–Baxter algebras, we can apply it to various MZV algebras to get identities there. We give some examples of such applications by using old and new results in Rota–Baxter algebras.

4.1. **Spitzer's identity.** Let (R, P) be a unitary commutative Rota–Baxter $\mathbb{Q}$-algebra of weight 1. Then for $a \in R$, we have the Spitzer's identity [38]

$$\exp\left(P(\log(1+at))\right) = \sum_{i=0}^{\infty} t^i \underbrace{P\big(P(P(\cdots P}_{i\text{-times}}(a)a)\cdots a)a\big) \tag{20}$$

in the ring of power series $R[[t]]$. We apply it to the MZV algebra of level 2 generated by A_H. For $k \geq 2$, let $a = f_k := 1/x^k \in A_H$. With the summation operator $P(f)(x) = \sum_{n\geq 1} f(x+n)$, we have

$$\begin{aligned} P(\log(1+at)) &= P\Big(\sum_{i=1}^{\infty} \frac{(-1)^{i-1}}{i}\left(\frac{t}{x^k}\right)^i\Big) \\ &= \sum_{i=1}^{\infty} \frac{(-1)^{i-1}}{i} P\left(\frac{1}{x^{ki}}\right) t^i \\ &= \sum_{i=1}^{\infty} \frac{(-1)^{i-1}}{i} \zeta(ki; x+1) t^i \end{aligned}$$

Similarly, the right hand side of Eq (20) becomes

$$1 + \sum_{i=1}^{\infty} \zeta(\underbrace{k, \cdots, k}_{i}; x+1)t^i.$$

So Evaluating at $x = 0$, we get the well-known identity

$$\exp\left(\sum_{i=1}^{\infty} (-1)^{i-1}\zeta(ik)\frac{t^i}{i}\right) = 1 + \sum_{i=1}^{\infty} \zeta(\underbrace{k, \cdots, k}_{i})t^i.$$

Applying Spitzer's identity to the subalgebra A_L gives similar relations of MPLs.

The non-commutative version of Spitzer's identity (20) gives Bogoliubov's formulae in perturbative renormalization of quantum field theory [23].

We now apply Spitzer's identity to the free Rota-Baxter algebra $A = Ш(\mathbb{C}[x])$ with its Rota-Baxter operator still denoted by P. For $u, v \in A$, define

$$u \star v = uP(v) + P(u)v + uv.$$

Then define

$$u^{\star n} = \underbrace{u \star \cdots \star u}_{n}, \quad \exp_\star(u) = \sum_{n\geq 0} u^{\star n}/n!.$$

We verify that $P(u)P(v) = P(u \star v)$ by definition of P and hence $P(u)^n = P(u^{\star n})$, $n \geq 1$. Using this to rewrite Spitzer's identity, the left hand side gives $P(\exp_\star \log(1+xt)) - P(1) + 1$. The right hand side gives

$$\begin{aligned} 1 + P(xt) + P(xtP(xt)) + \cdots &= 1 + 1 \otimes xt + 1 \otimes xt \otimes xt + \cdots \\ &= P(1 + xt + (xt)^{\otimes 2} + \cdots) - P(1) + 1. \end{aligned}$$

Thus $\exp_* \log(1+xt) = 1 + xt + (xt)^{\otimes 2} + \cdots$. This is a basic identity in [34].

4.2. **Bohnenblust-Spitzer formula.** We quote the following theorem that first appeared in the same paper [44] where Spitzer published his above formula and takes it present form in [40].

Theorem 4.1. (Bohnenblust-Spitzer formula) *Let A be a Rota–Baxter algebra. Then*

$$\sum_{\sigma\in S_n} P(s_{\sigma(1)}P(s_{\sigma(2)}\cdots P(s_{\sigma(n)})\cdots)) = \sum_{\mathfrak{T}} (-1)^{n-|\mathfrak{T}|} \prod_{T\in\mathfrak{T}} (|T|-1)! P(\prod_{j\in T} s_j), \ n > 0.$$

Here $s_j > 1, 1 \leq j \leq n$ and $\mathfrak{T}$ runs through all unordered set partitions of $\{1, \cdots, n\}$.

Applying this identity to A_H, we obtain an identity of multiple Hurwitz zeta functions. Then specialized at $x = 0$, we have the following important Partition Identity of Hoffman [32].

Corollary 4.2. *For $s_i > 1$, $1 \leq i \leq n$, we have*

$$\sum_{\sigma\in S_n} \zeta(s_{\sigma(1)}, \cdots, s_{\sigma(n)}) = \sum_{\mathfrak{T}} (-1)^{n-|\mathfrak{T}|} \prod_{T\in\mathfrak{T}} (|T|-1)! \zeta(\sum_{j\in T} s_j), \ n > 0.$$

For example, when $n = 2$, we have the identity

$$P(s_1P(s_2)) + P(s_2P(s_1)) = -P(s_1s_2) + P(s_1)P(s_2),$$

in Rota–Baxter algebras, translated to

$$\zeta(s_1, s_2) + \zeta(s_2, s_1) = -\zeta(s_1 + s_2) + \zeta(s_1)\zeta(s_2).$$

Applying Bohnenblust-Spitzer formula to A_q, we have the q-analog of Hoffman's identity proved by Bradley [8].

4.3. **Congruences.** The following congruence relation is prove in [27].

Theorem 4.3. *Let p be a prime number. For any $a_1\otimes\cdots\otimes a_n \in A^{\otimes n}$ in the free Rota-Baxter algebra $Ш(A)$, we have*

$$\text{(Tensor/Graduate form of Freshman's Dream)} \quad (a_1 \otimes \cdots \otimes a_n)^p \equiv a_1^p \otimes \cdots \otimes a_n^p \mod p$$

in the sense that p divides the coefficients of all other pure tensors when the power on the left hand side is expressed as a linear combination of pure tensors. Here the product on the left hand side is the product in $Ш(A)$ defined in Eq (7).

Compare with the well-known Freshman's Dream

$$(x+y)^p \equiv x^p + y^p \mod p.$$

Applying the theorem to the MZV algebra A_H of multiple Hurwitz series and evaluating at $x = 0$, we have

Corollary 4.4.

$$\zeta(s_1, \cdots, s_n)^p \equiv \zeta(ps_1, \cdots, ps_n) \mod p$$

in the sense that the coefficients of all other multiple zeta values on the right hand side is a multiple of p*.*

Similar congruences hold for MPLs.

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